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ABSTRACT OR SUPPORTING INFORMATION

Presentation/Publication Information:

An invited talk to be given by Deepak Srivastava of the Computational Nanotechnology task at the monthly Silicon Valley Computer Club gathering on 17th March, 1999 at 8, Almandra Lane, Los Altos, CA.

A copy of the presentation is attached.

Acknowledgments:

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Abstract:

An invited talk to review the status of the progress in Nanotechnology, based on publicly available, already presented and/or published material. The copy of the slides are enclosed. No abstract was required or submitted for this presentation.

Carbon based Nanotechnology: Review

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Rod Ruoff –– University of Washington, St. Louis
K. J. Cho –– Stanford University

Review of Carbon Nanotechnology: in context of Drexler's Molecular Nanotechnology.

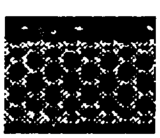
- Concept: Feynman's postulate
- Vision: Molecular Assemblers
- Progress in Microtechnology

Research Focus

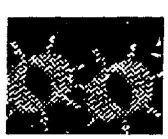
Nano-mechanics/materials

Carbon based electronics

Nanodevice /Materials Applications



BxCyNz Nanotubes



Nanotube–Motor

Nano-lithography

H2 Storage in nanotubes

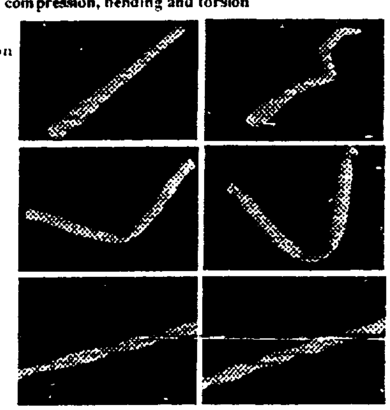
Nanotube – Nanomechanics

- **Nanotubes are extremely strong highly elastic nanofibers**
  – high value of Young modulus swnt – 1.2 TPa
- **Dynamic response of nanotubes to ballistic deformation**
  – axial compression, bending and torsion

Axial Compression

Bending

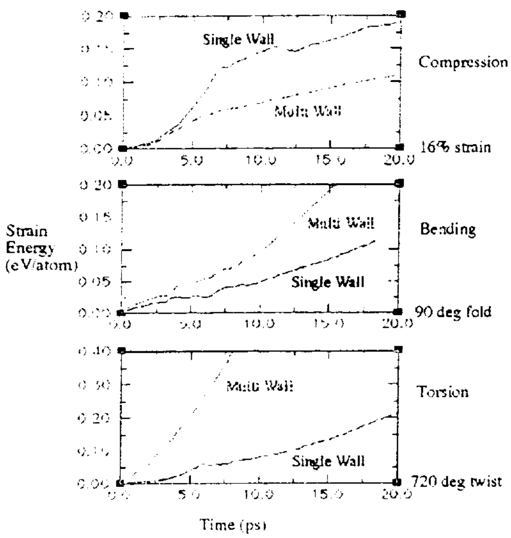
Torsion



– redistribution of strain
– sharp buckling leading to bond rupture

Nanotube– Nanomechanics

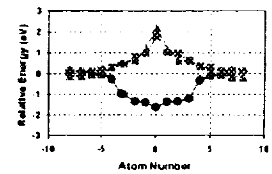
Energetics of Mechanical Deformation

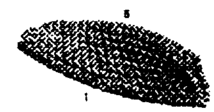


Nano Mechano–Chemistry I

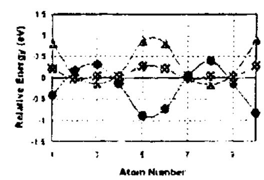
- Predictions of enhanced chemical reactivity in regions of local conformational strains: Kinky Chemistry

Kink on a bent tubule



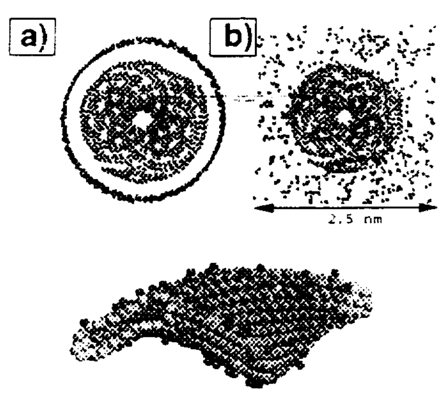


Ridge on a twisted tubule



Binding Energy
Cohesive Energy
Electronic Energy

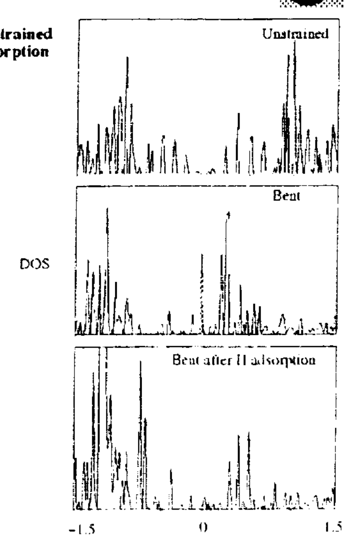
Nano Mechano–Chemistry II



Torsionally twisted SWNT equilibrated in an H bath

Nano Mechano–Chemistry III

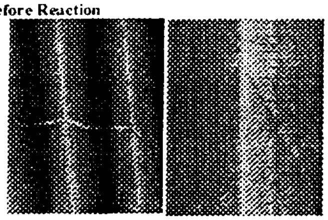
- Mechanism of Strained induced chemisorption



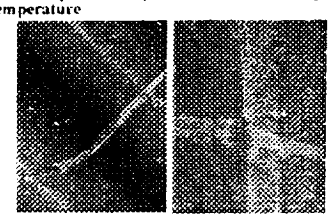
Nano Mechano–Chemistry III

SEM images of MWNTs dispersed on a V- ridge substrate

(a) Before Reaction



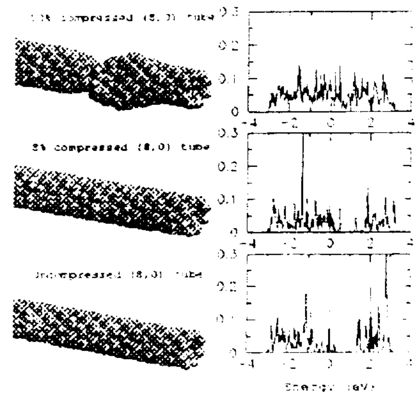
(b) Same sample after exposure to nitric acid vapor at room temperature



"Predictions of enhanced chemical reactivity in regions of local conformational strains: kinky chemistry," D. Srivastava, J. D. Schall, D. W. Brenner, K. D. Ausman M. Feng, and R. Ruoff, submitted, J. Phys. Chem (1999).

Nano Mechano–Electronics I

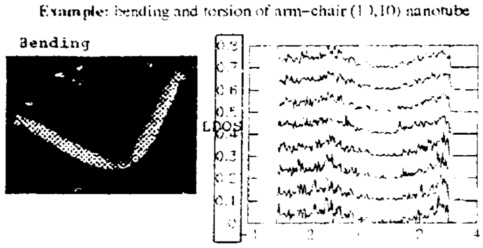
- Mechanical deformations alter the Electronic Characteristics of Nanotubes

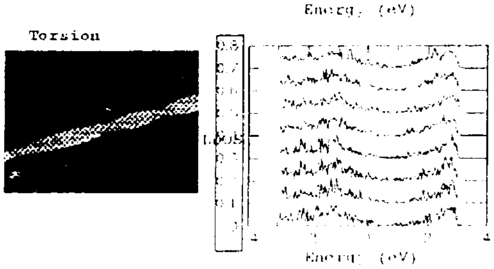


Nano mechano–electronics effects are "strongly" dependent on tube chiralities."

Nano Mechano–Electronics II

Example: bending and torsion of arm–chair (10,10) nanotube





Research Focus II
Carbon based Electronics

Experimental Status

Individual Single Wall Nanotubes as Quantum Wire

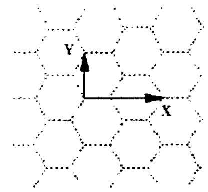
S. J. Tans et. al, Nature (April, 97)

- **Nanotube Nanodevice – showing localized rectifying behavior in the I/V characteristics**
  P. G. Collins et. al., Science (October, 97)
- **I/V Characteristics and Electronic Structure (DOS) of structurally nanotubes.**
  J W G Wildoer et. al., Nature (January, 98)
  T. W. Odom et. al., Nature (January, 98)
- **Single nanotube–molecule transistor at room temp.**
  S. J. Tans et. al. (Nature) (May, 98)
- **Nanostructuring (cutting) of nanotubes with STM**
  L. C. Venema et. al., Appl. Phys. Lett. (Nov, 97)

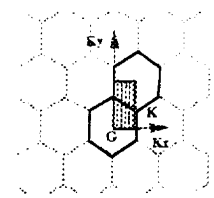
CxByNz Nanotubes: Nano-Electronics
Nano-mechanics

- molecular wires
- Topological defect mediated Hetero-junctions ~ switching
  transisting
  tunneling devices
- Nano Mechano-Chemistry
  Site-specific chemical functionalization
  Hetero-junctions
- Nano Mechano-Electronics
- C nanotubes doped with B and N
  Heteroatomic CxByNz nanotubes
  Heterojunctions
  Superlattices

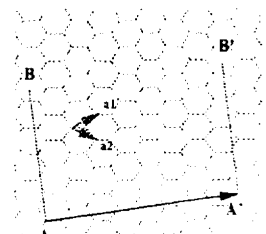
Carbon Nanotube Electronics Band Structure (basics)



Hexagonal Lattice of a Graphene Sheet - (2xunit cell)

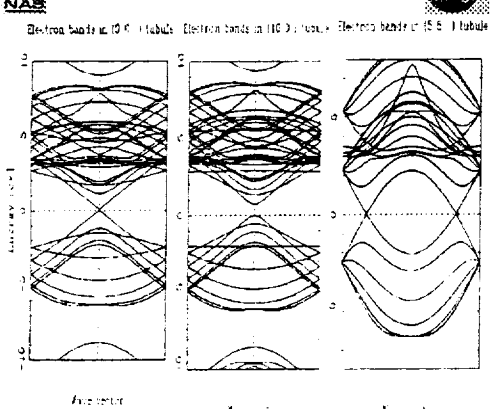


First Brillouin zone for an arm-chair tube.



Ch = n a1 + m a2 (chiral vector)

Carbon Nanotube Electronics Band Structure



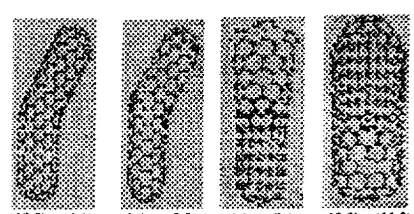
(9,0) tube (10,0) tube (5,5) tube

Arm chair tubes (n,n) ~ metal like

Otherwise m-n = 3I (I integer) metal like

Topological Defect: HeteroJunctions I

2- point Nanotube Heterojunctions
Molecular Electronic Switches



(10,0) - (6,6) (9,0) - (5,5) (8,0) - (7,1) (12,0) - (11,0)

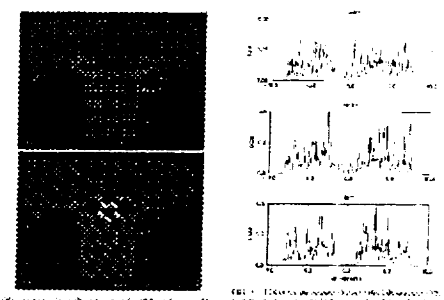
Bent Junctions Straight Junctions

Semiconductor-Metal
Semimetal-Metal

Chico et. al. Phys. Rev. Lett., 96
Charlier et. al. Phys. Rev. B, 96
Lambine et. al. Chem. Phys. Lett., 96
Saito et. al. Phys. Rev. B, 96

We studied the effect of capping the tubes and relaxing the junctions with a quantum GTBMD method.

Topological Defect: HeteroJunctions II

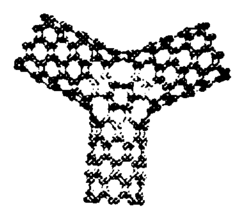


LDOS of (10,0)-(9,0) "T-junction"

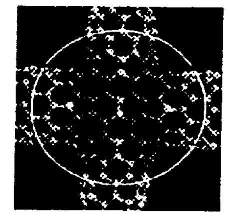
3-terminal "T-tunnel" Junctions of Nanotubes

Topological Defects: Heterojunctions III

Pathways to Three-Dimensional Molecular "Networks"



Metal-Semiconductor-Metal "Y" Tunnel Junction



A four-terminal nanotube heterojunction

"It turns out that all of our proposed junctions satisfy - Generalized Euler's Rule about the global topology of connected networks"

– V. Crespi, Phys. Rev. Lett. (98)

These are "ideal" junctions and we dont know how to make these !

Some work is in progress to conceptualize and test "real" junctions.

CxByNz Nanotubes and Junctions I

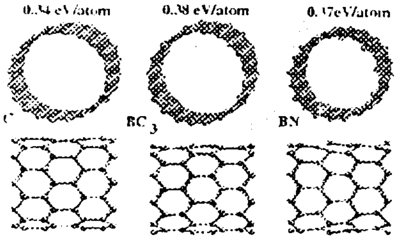
- Band gap engineering over a larger range should be possible:

BN	~ 5.5 eV
BC_2N	~ 2.0 eV
C	~ 0 - 1 eV
BC_3	~ 0.5 eV

  - a variety of junctions, quantum dots and superlattices should be possible
  - should be more robust

- Example: Composite (10,0) nanotube

0.34 eV/atom   0.38 eV/atom   0.37eV/atom

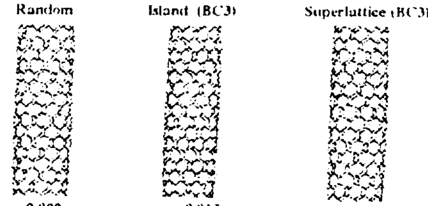


reconstruction due to polar BN bond

CxByNz Nanotubes and Junctions II

- B doping of Carbon Nanotube

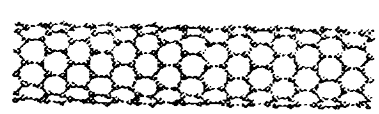
Random   Island (BC3)   Superlattice (BC3)



0.000   -0.013   -0.016 eV/atom

phase separation of doped and undoped regions is thermodynamically stable !

- BN/C Junctions

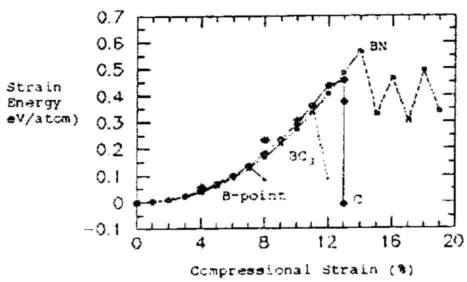


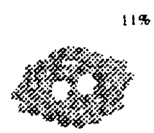
Interface Energy = 2*BN/C - BN - C
Interface Energy = 0.33eV/CB bond

Stable interfaces should be possible !

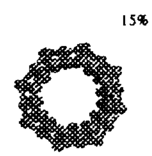
Cx By Nz Nanotubes and Junctions III

Nano–mechanics of Composite Nanotubes (8,0)





Structurally collapsed C nanotube



Structurally collapsed BN nanotube

Comments:

Proposed "new" nanotechnology materials and devices.

- **multiple nanotube junctions and networks**
- **B, N doping, interfaces and tips**

Tested feasibility of "new" concepts:

- **Conformational strain driven mechanical – kinky – chemistry is certainly a new way to do site specific reactions on side–walls.**
- **feasibility of H storage in nanotube based material**

Future possibilities are bright: